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Non-smooth and Complementarity-based Distributed Parameter Systems: Simulation and Hierarchical Optimization

Preprint Number SPP1962-099

received on November 6, 2018

Edited by SPP1962 at Weierstrass Institute for Applied Analysis and Stochastics (WIAS) Leibniz Institute in the Forschungsverbund Berlin e.V. Mohrenstraße 39, 10117 Berlin, Germany E-Mail: spp1962@wias-berlin.de

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# GRADIENT-BASED SOLUTION ALGORITHMS FOR A CLASS OF BILEVEL OPTIMIZATION AND OPTIMAL CONTROL PROBLEMS WITH A NON-SMOOTH LOWER LEVEL\*

# CONSTANTIN CHRISTOF<sup>†</sup>

Abstract. The aim of this paper is to explore a peculiar regularization effect that occurs in the sensitivity analysis of certain elliptic variational inequalities of the second kind. The effect causes the solution operator of the variational inequality at hand to be continuously Fréchet differentiable although the problem itself contains non-differentiable terms. Our analysis shows in particular that standard gradient-based algorithms can be used to solve bilevel optimization and optimal control problems that are governed by elliptic variational inequalities of the considered type - all without regularizing the non-differentiable terms in the lower-level problem and without losing desirable properties of the solution as, e.g., sparsity. Our results can, for instance, be used in the optimal control of Casson fluids and in bilevel optimization approaches for parameter learning in total variation image denoising models.

Key words. optimal control, non-smooth optimization, bilevel optimization, elliptic variational inequality of the second kind, Casson fluid, total variation, machine learning, parameter identification

AMS subject classifications. 49J40, 49J52, 49N45, 68U10, 76A05, 90C33

1. Introduction and Problem Statement. The aim of this paper is to study finite-dimensional optimization problems of the type

(P) 
$$\begin{cases} \min J(y, u, \alpha, \beta) \\ \text{s.t. } y, u \in \mathbb{R}^n, \ \alpha, \beta \in \mathbb{R}^m, \ (u, \alpha, \beta) \in U_{ad}, \\ \langle A(y), v - y \rangle + \sum_{k=1}^m \omega_k (\alpha_k \|G_k v\| + \beta_k \|G_k v\|^{1+\gamma}) \\ - \sum_{k=1}^m \omega_k (\alpha_k \|G_k y\| + \beta_k \|G_k y\|^{1+\gamma}) \ge \langle Bu, v - y \rangle \ \forall v \in \mathbb{R}^n. \end{cases}$$

Our standing assumptions on the quantities in (P) are as follows:

ASSUMPTION 1.1. (Standing Assumptions and Notation)

- 1.  $l, m, n \in \mathbb{N}, \omega \in (0, \infty)^m, B \in \mathbb{R}^{n \times n}$  and  $\gamma \in (0, 1)$  are given and fixed,
- 2.  $G_k \in \mathbb{R}^{l \times n}$ , k = 1, ..., m, are given matrices,
- 3.  $J: \mathbb{R}^n \times \mathbb{R}^n \times \mathbb{R}^m \times \mathbb{R}^m \to \mathbb{R}$  is a continuously Fréchet differentiable function,
- 4.  $U_{ad}$  is a (sufficiently nice) non-empty subset of  $\mathbb{R}^n \times [0,\infty)^m \times (0,\infty)^m$ ,
- 5.  $A: \mathbb{R}^n \to \mathbb{R}^n$  is a continuously Fréchet differentiable operator that is strongly monotone, i.e., there is a constant c > 0 with

$$\langle A(v_1) - A(v_2), v_1 - v_2 \rangle \ge c \|v_1 - v_2\|^2 \qquad \forall v_1, v_2 \in \mathbb{R}^n,$$

6.  $\|\cdot\|$  denotes the Euclidean norm and  $\langle\cdot,\cdot\rangle$  the Euclidean scalar product (we use the same symbol on  $\mathbb{R}^l$ ,  $\mathbb{R}^m$  and  $\mathbb{R}^n$ ).

<sup>\*</sup>Submitted to the editors DATE.

Funding: This research was conducted within the International Research Training Group IGDK 1754, funded by the German Science Foundation (DFG) and the Austrian Science Fund (FWF), and in association with project P16 of SPP 1962 "Non-Smooth and Complementarity-Based Distributed Parameter Systems: Simulation and Hierarchical Optimization".

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Note that, if the operator  $A : \mathbb{R}^n \to \mathbb{R}^n$  can be identified with the gradient field of a convex and Fréchet differentiable function  $a : \mathbb{R}^n \to \mathbb{R}$ , i.e., if  $a'(v) = A(v) \in \mathbb{R}^n$ holds for all  $v \in \mathbb{R}^n$ , then (P) is equivalent to the bilevel minimization problem

(1.1) 
$$\begin{cases} \min J(y, u, \alpha, \beta) \\ \text{s.t. } y, u \in \mathbb{R}^n, \ \alpha, \beta \in \mathbb{R}^m, \ (u, \alpha, \beta) \in U_{ad}, \\ y = \underset{v \in \mathbb{R}^n}{\operatorname{arg\,min}} a(v) + \sum_{k=1}^m \omega_k \Big( \alpha_k \|G_k v\| + \beta_k \|G_k v\|^{1+\gamma} \Big) - \langle Bu, v \rangle \,. \end{cases}$$

For a proof of this equivalence, we refer to [10, Section 1.2]. Since elliptic variational inequalities involving non-conservative vector fields  $A : \mathbb{R}^n \to \mathbb{R}^n$  appear naturally in some applications (cf. the references in [24, Section II-2.1]), we work with the more general formulation (P) in this paper and not with (1.1).

Optimization problems of the type (P) arise, for instance, in the optimal control of non-Newtonian fluids, in glaciology, and in bilevel parameter learning approaches for variational image denoising models. See, e.g., [6, 7, 8, 15, 17, 18, 20, 21, 25, 26, 28, 30, 31, 32, 33, 35, 36] and the references therein, and also the two tangible examples in Section 2. The main difficulty in the study of the problem (P) is the nonsmoothness of the Euclidean norms present on the lower level. Because of these nondifferentiable terms, standard results and solution methods are typically inapplicable, and the majority of authors resorts to regularization techniques to determine, e.g., stationary points of (P), cf. the approaches in [8, 15, 20, 28, 36].

The aim of this paper is to demonstrate that, in the situation of Assumption 1.1, problems of the type (P) can also be solved without replacing the involved Euclidean norms with smooth approximations. To be more precise, in what follows, we prove the rather surprising fact that the solution operator  $S: (u, \alpha, \beta) \mapsto y$  associated with the inner elliptic variational inequality in (P) is continuously Fréchet differentiable as a function  $S: \mathbb{R}^n \times [0, \infty)^m \times (0, \infty)^m \to \mathbb{R}^n$  (see Theorem 3.3 for the main result). This very counterintuitive behavior makes it possible to tackle minimization problems of the type (P) with gradient-based solution algorithms, even without regularizing the non-smooth terms on the lower level. Avoiding such a regularization is highly desirable in many situations as the Euclidean norms in (P) typically cause the inner solutions y to have certain properties (sparsity etc.) that are very important from the application point of view. Before we begin with our investigation, we give a short overview of the content and the structure of this paper:

In Section 2, we first give two tangible examples of problems that fall under the scope of our analysis - one arising in the optimal control of non-Newtonian fluids and one from the field of bilevel parameter learning in variational image denoising models. The examples found in this section illustrate that our results are not only of academic interest but also of relevance in practice. In Section 3, we then address the sensitivity analysis of the inner elliptic variational inequality in (P). Here, we prove that the solution operator  $S : (u, \alpha, \beta) \mapsto y$  is indeed continuously Fréchet differentiable as a function  $S : \mathbb{R}^n \times [0, \infty)^m \times (0, \infty)^m \to \mathbb{R}^n$  and also give some comments, e.g., on the extension of our results to the infinite-dimensional setting. Section 4 is concerned with the consequences that the results of Section 3 have for the study and the numerical solution of bilevel optimization problems of the form (P). Lastly, in Section 5, we demonstrate by means of a numerical example that the differentiability of the solution map S indeed allows to solve problems of the type (P) with standard gradient-based algorithms.

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2. Two Application Examples. In what follows, we discuss in more detail two application examples that are covered by the general problem formulation (P) and that may serve as a motivation for the analysis in Sections 3 and 4.

**2.1. Optimal Control of Casson Fluids.** As a first example, we consider a problem that arises in the optimal control of non-Newtonian fluids: Suppose that  $\Omega \subset \mathbb{R}^d$ ,  $d \in \{1, 2\}$ , is a simply-connected, bounded, polyhedral domain, let  $L^p(\Omega)$ ,  $1 \leq p \leq \infty$ , and  $H_0^1(\Omega)$  be defined as usual (see [1, 3] or other standard references), and let  $(\bar{u}, \alpha) \in L^2(\Omega) \times (0, \infty)$  be arbitrary but fixed. Then, the so-called Mosolov problem for Casson fluids is given by

(2.1) 
$$\bar{y} = \underset{\bar{v} \in H_0^1(\Omega)}{\operatorname{arg\,min}} \int_{\Omega} \frac{1}{2} \|\nabla \bar{v}\|^2 + \frac{4}{3} \alpha^{1/2} \|\nabla \bar{v}\|^{3/2} + \alpha \|\nabla \bar{v}\| - \bar{u} \bar{v} \, \mathrm{d}x.$$

Here,  $\nabla$  denotes the weak gradient, and the bars indicate that we talk about functions and not about elements of the Euclidean space. In non-Newtonian fluid mechanics, the main interest in the minimization problem (2.1) stems from the fact that it models the unidirectional, stationary flow of a viscoplastic medium of Casson type between two plates with distance diam( $\Omega$ ) in the case d = 1 and in a cylindrical pipe with cross-section  $\Omega$  in the case d = 2, cf. [26, 31, 32, 33] and the references therein. In this context,  $\bar{u}$  is the pressure gradient parallel to the two enclosing plates/the pipe axis driving the fluid,  $\bar{y}$  is the fluid velocity in the direction of  $\bar{u}$  (i.e., perpendicular to  $\Omega$ ), and  $\alpha$  is a material parameter (the generalized Oldroyd number), see Figure 1 below. Recall that the characteristic feature of a viscoplastic medium is that it behaves like a fluid everywhere where the shear stress exceeds a certain threshold (the so-called yield stress) and that it behaves like a solid otherwise. For a Casson fluid, the behavior in fluid regions is additionally governed by a non-linear relation between the shear rate and the shear stress, cf. [26, Section 2.2]. In the model (2.1), the regions where rigid material behavior occurs are precisely those parts of the domain  $\Omega$  where the gradient  $\nabla \bar{y}$  vanishes, and the sudden change of the material behavior at the yield stress and the non-linear material laws in the fluid regions are incorporated via the terms  $\int_{\Omega} \alpha \|\nabla \bar{v}\| dx$  and  $\int_{\Omega} \frac{1}{2} \|\nabla \bar{v}\|^2 + \frac{4}{3} \alpha^{1/2} \|\nabla \bar{v}\|^{3/2} dx$ , respectively, see the derivation in [26, Section 2]. Note that this implies in particular that the non-differentiability of the objective in (2.1) is directly related to the underlying physical model, and that the non-smoothness is of special importance in the above situation.



FIG. 1. Typical flow behavior in the situation of the two-dimensional Mosolov problem with a constant pressure drop  $\bar{u}$ . The viscoplastic medium forms a solid nucleus in the middle of the fluid domain that moves with a constant velocity c along the pipe axis and sticks to the boundary in those regions of  $\Omega$  where the pressure gradient  $\bar{u}$  is too low to move the fluid (so-called stagnation zones). An analogous behavior can be observed in the case d = 1 for the flow of a Casson fluid between two plates, cf. the numerical results in Section 5.

Suppose now that we want to determine a pressure gradient  $\bar{u} \in L^2(\Omega)$  and a material parameter  $\alpha \in (0, \infty)$  such that the flow profile  $\bar{y} \in H_0^1(\Omega)$  in  $\Omega$  has a certain shape  $\bar{y}_D \in C(\operatorname{cl}(\Omega)) \cap H_0^1(\Omega)$ , where  $C(\operatorname{cl}(\Omega))$  denotes the space of continuous functions on the closure of the domain  $\Omega$ . Then, it is a natural approach to consider a tracking-type optimal control problem of the form

(2.2) 
$$\begin{cases} \min \frac{1}{2} \|\bar{y} - \bar{y}_D\|_{L^2(\Omega)}^2 + \frac{\mu}{2} \left( \|\bar{u}\|_{L^2(\Omega)}^2 + \alpha^2 \right) \\ \text{s.t.} \quad \bar{y} \in H_0^1(\Omega), \ \bar{u} \in L^2(\Omega), \ \alpha \in \tilde{U}_{ad}, \\ \bar{y} = \operatorname*{arg\,min}_{\bar{v} \in H_0^1(\Omega)} \int_{\Omega} \frac{1}{2} \|\nabla \bar{v}\|^2 + \frac{4}{3} \alpha^{1/2} \|\nabla \bar{v}\|^{3/2} + \alpha \|\nabla \bar{v}\| - \bar{u}\bar{v} \, \mathrm{d}x, \end{cases}$$

where  $\tilde{U}_{ad}$  is some non-empty, convex and closed subset of  $(0, \infty)$  and where  $\mu > 0$  is a fixed Tychonoff parameter. Let us briefly check that the above problem is indeed sensible:

THEOREM 2.1 (Solvability of (2.2)). Assume that  $\bar{y}_D$ ,  $\Omega$ ,  $\mu$  and  $\tilde{U}_{ad}$  are as before. Then, (2.2) admits at least one solution  $(\bar{u}^*, \alpha^*) \in L^2(\Omega) \times \tilde{U}_{ad}$ .

Proof. From standard arguments (as found, e.g., in [24, Lemma 4.1]), it follows straightforwardly that the lower-level problem in (2.2) possesses a well-defined solution operator  $S: L^2(\Omega) \times [0, \infty) \to H_0^1(\Omega), (\bar{u}, \alpha) \mapsto \bar{y}$ . It is further easy to check (using the weak lower semicontinuity of convex and continuous functions) that this solution map is weak-to-weak continuous, i.e., for every sequence  $\{(\bar{u}_i, \alpha_i)\} \subset L^2(\Omega) \times [0, \infty)$ with  $\bar{u}_i \to \bar{u}$  in  $L^2(\Omega)$  and  $\alpha_i \to \alpha$  in  $\mathbb{R}$  for  $i \to \infty$ , we have  $S(\bar{u}_i, \alpha_i) \to S(\bar{u}, \alpha)$ in  $H_0^1(\Omega)$ . The claim now follows immediately from the direct method of calculus of variations and the compactness of the embedding  $H_0^1(\Omega) \hookrightarrow L^2(\Omega)$ .

To transform (2.2) into a problem that can be solved numerically, we consider a standard finite element discretization with piecewise linear ansatz functions. More precisely, we assume the following:

ASSUMPTION 2.2. (Assumptions and Notation for the Discretization of (2.2)) 1.  $\mathcal{T} = \{T_k\}_{k=1}^m, m \in \mathbb{N}, \text{ is a triangulation of } \Omega \text{ consisting of simplices } T_k \text{ (see,}$ 

- e.g., [9, Definition 2] for the precise definition of the term "triangulation"),  $[2, [n]^n$   $n \in \mathbb{N}$  are the nodes of  $\mathcal{T}$  that are contained in  $\Omega$
- 2.  $\{x_i\}_{i=1}^n$ ,  $n \in \mathbb{N}$ , are the nodes of  $\mathcal{T}$  that are contained in  $\Omega$ ,
- 3.  $V_h := \{ \bar{v} \in C(\operatorname{cl}(\Omega)) \mid \bar{v} \text{ is affine on } T_k \text{ for all } k = 1, ..., m \text{ and } \bar{v}|_{\partial\Omega} = 0 \},$
- 4.  $\{\varphi_i\}$  is the nodal basis of  $V_h$ , i.e.,  $\varphi_i(x_i) = 1$  for all  $i, \varphi_i(x_j) = 0$  for  $i \neq j$ .

By replacing the spaces  $H_0^1(\Omega)$  and  $L^2(\Omega)$  in (2.2) with  $V_h$ , we now arrive at a finite-dimensional minimization problem of the following form: (2.3)

$$\begin{cases} \min \frac{1}{2} \langle B(y - y_D), y - y_D \rangle + \frac{\mu}{2} \left( \langle Bu, u \rangle + \alpha^2 \right) \\ \text{s.t.} \quad y, u \in \mathbb{R}^n, \ \alpha \in \tilde{U}_{ad}, \\ y = \operatorname*{argmin}_{v \in \mathbb{R}^n} \frac{1}{2} \langle Av, v \rangle + \sum_{k=1}^m |T_k| \left( \alpha \|G_k v\| + \frac{4}{3} \alpha^{1/2} \|G_k v\|^{3/2} \right) - \langle Bu, v \rangle. \end{cases}$$

Here, y, u and  $y_D$  are the coordinate vectors of the discretized state, the discretized control and the Lagrange interpolate of  $\bar{y}_D$  w.r.t. the nodal basis  $\{\varphi_i\}$ , respectively,

A and B denote the stiffness and the mass matrix, i.e.,

$$A := \left( \int_{\Omega} \left\langle \nabla \varphi_i, \nabla \varphi_j \right\rangle \mathrm{d}x \right)_{i,j=1,\dots,n}, \qquad B := \left( \int_{\Omega} \varphi_i \varphi_j \mathrm{d}x \right)_{i,j=1,\dots,n}$$

 $|T_k|$  is the *d*-dimensional volume of the simplex  $T_k$ , and  $G_k \in \mathbb{R}^{d \times n}$  is the matrix that maps a coordinate vector  $v \in \mathbb{R}^n$  to the gradient of the associated finite element function on the cell  $T_k$ , i.e.,

$$G_k v = \nabla \left( \sum_{i=1}^n v_i \varphi_i \right) \bigg|_{T_k} \in \mathbb{R}^d \qquad \forall v \in \mathbb{R}^n \qquad \forall k = 1, ..., m.$$

Note that (2.3) is precisely of the form (1.1) (with  $\omega_k := |T_k|$  and an appropriately defined  $U_{ad} \subset \mathbb{R}^n \times [0, \infty)^m \times (0, \infty)^m$ ). This shows that, after a discretization, the minimization problem (2.2) indeed falls under the scope of the general setting introduced in Section 1, and that our analysis indeed allows to study optimal control problems for Casson fluids. We will get back to this topic in Section 5, where (2.3) will serve as a model problem for our numerical experiments.

2.2. Bilevel Optimization Approaches for Parameter Learning. As a second application example, we consider a bilevel optimization problem that has been proposed in [28] as a framework for parameter learning in variational image denoising models (cf. also with [6, 36]). The problem takes the form

(2.4) 
$$\begin{cases} \min \|y - g\|^2 \\ \text{s.t. } y \in \mathbb{R}^n, \ \vartheta \in [0, \infty)^q, \\ y = \operatorname*{argmin}_{v \in \mathbb{R}^n} \frac{1}{2} \|v - f\|^2 + \sum_{i=1}^q \vartheta_i \left( \sum_{j=1}^r |(K_i v)_j|^p \right). \end{cases}$$

Here, n, q and r are natural numbers, p is some exponent in  $[1, \infty)$ ,  $g \in \mathbb{R}^n$  is the given ground truth data, f is the noisy image, the terms  $\sum_{j=1}^r |(K_i v)_j|^p$ , i = 1, ..., q, are socalled analysis-based priors involving matrices  $K_i \in \mathbb{R}^{r \times n}$ ,  $\vartheta$  is the learning parameter, and  $\frac{1}{2} ||v - f||^2$  and  $\sum_{i=1}^q \vartheta_i (\sum_{j=1}^r |(K_i v)_j|^p)$  are the fidelity and the regularization term of the underlying denoising model, respectively (cf. the classical TV-denoising method). For more details on the background of (2.4), we refer to [28] and the references therein.

Suppose now that we enrich the model (2.4) by allowing the exponent p to depend on i and by doubling the number of priors in the lower-level problem. Then, we may choose half of the exponents p to be one and half of the exponents p to be  $1 + \gamma$  for some  $\gamma \in (0, 1)$  to arrive at a problem of the type (2.5)

$$\begin{cases} \min \|y - g\|^2 \\ \text{s.t. } y \in \mathbb{R}^n, \ \vartheta, \tilde{\vartheta} \in [0, \infty)^q, \\ y = \operatorname*{argmin}_{v \in \mathbb{R}^n} \frac{1}{2} \|v - f\|^2 + \sum_{i=1}^q \vartheta_i \left( \sum_{j=1}^r |(K_i v)_j| \right) + \tilde{\vartheta}_i \left( \sum_{j=1}^r |(K_i v)_j|^{1+\gamma} \right). \end{cases}$$

Note that it makes sense to consider the exponent p = 1 here since this choice ensures that the priors are sparsity promoting (due to the induced non-smoothness, cf. [41]).

If we replace the constraint on  $\tilde{\vartheta}$  in (2.5) with  $\tilde{\vartheta} \in [\varepsilon, \infty)^q$  for some  $0 < \varepsilon \ll 1$ , define

(2.6) 
$$\alpha_{ij} := \vartheta_i, \qquad \beta_{ij} := \tilde{\vartheta}_i, \qquad G_{ij} : \mathbb{R}^n \to \mathbb{R}, \quad v \mapsto (K_i v)_j,$$

use the binomial identities, exploit that terms which depend only on f are irrelevant in the lower-level problem, and identify f with u, then (2.5) can be recast as

$$\min \|y - g\|^2$$
  
s.t.  $y, u \in \mathbb{R}^n, \ \alpha, \beta \in \mathbb{R}^{rq}, \ (u, \alpha, \beta) \in U_{ad},$ 
$$y = \operatorname*{argmin}_{v \in \mathbb{R}^n} \frac{1}{2} \|v\|^2 + \sum_{i=1}^q \sum_{j=1}^r \alpha_{ij} |G_{ij}v| + \beta_{ij} |G_{ij}v|^{1+\gamma} - \langle u, v \rangle$$

with an appropriately defined admissible set  $U_{ad} \subset \mathbb{R}^n \times [0, \infty)^{rq} \times (0, \infty)^{rq}$  which ensures the equality u = f and enforces that  $\alpha_{ij}$  and  $\beta_{ij}$  depend only on i (cf. (2.6)). The above problem is again of the form (1.1) and satisfies all conditions in Assumption 1.1. This shows that the general setting of Section 1 can also be used to study parameter learning problems for variational image denoising models.

**3.** Solvability and Sensitivity Analysis of the Inner Problem in (P). Having demonstrated that the general framework of Section 1 indeed covers situations that are relevant for practical applications, we now turn our attention to the inner elliptic variational inequality in (P), i.e., to the problem

(V) 
$$\begin{cases} y \in \mathbb{R}^n, \\ \langle A(y), v - y \rangle + \sum_{k=1}^m \omega_k \left( \alpha_k \| G_k v \| + \beta_k \| G_k v \|^{1+\gamma} \right) \\ - \sum_{k=1}^m \omega_k \left( \alpha_k \| G_k y \| + \beta_k \| G_k y \|^{1+\gamma} \right) \ge \langle Bu, v - y \rangle \quad \forall v \in \mathbb{R}^n. \end{cases}$$

Here and in what follows, we always assume that  $l, m, n, \omega, B, \gamma, G_k$  and A satisfy the conditions in Assumption 1.1. Let us first check that (V) is well-posed:

PROPOSITION 3.1 (Solvability). The variational inequality (V) admits a unique solution  $y \in \mathbb{R}^n$  for all  $u \in \mathbb{R}^n$ ,  $\alpha \in [0, \infty)^m$  and  $\beta \in [0, \infty)^m$ . This solution satisfies

(3.1) 
$$\begin{cases} \langle A(y), z \rangle + \sum_{k=1}^{m} \omega_k \Big( \alpha_k \| \cdot \|'(G_k y; G_k z) + \beta_k (\| \cdot \|^{1+\gamma})'(G_k y; G_k z) \Big) \ge \langle Bu, z \rangle \\ \forall z \in \mathbb{R}^n, \end{cases}$$

where H'(x;h) denotes the directional derivative of a function  $H : \mathbb{R}^l \to \mathbb{R}$  at a point  $x \in \mathbb{R}^l$  in a direction  $h \in \mathbb{R}^l$ . Further, there exists a constant C > 0 independent of  $u, \alpha$  and  $\beta$  with  $||y|| \leq C||u||$  for all  $u, \alpha$  and  $\beta$ .

*Proof.* The unique solvability of (V) for all  $u \in \mathbb{R}^n$ ,  $\alpha \in [0, \infty)^m$  and  $\beta \in [0, \infty)^m$  is a straightforward consequence of Browder's theorem, see [40, Theorem 3.43] and [10, Theorem 1.2.2]. To obtain the variational inequality (3.1), it suffices to choose vectors of the form v = y + tz, t > 0,  $z \in \mathbb{R}^n$ , in (V), to divide by t, and to pass to the limit  $t \searrow 0$ . The bound  $||y|| \le C||u||$  finally follows from (V) when we choose v = 0 and exploit the strong monotonicity of A.

As a starting point for our sensitivity analysis, we prove:

PROPOSITION 3.2 (Lipschitz Continuity of the Solution Map). For every M > 0there exists a constant C > 0 depending only on  $\omega$ , M, A, B and  $G_k$  such that the solution map  $S : \mathbb{R}^n \times [0, \infty)^m \times [0, \infty)^m \to \mathbb{R}^n$ ,  $(u, \alpha, \beta) \mapsto y$ , associated with (V) satisfies

(3.2) 
$$\|S(u_1,\alpha_1,\beta_1) - S(u_2,\alpha_2,\beta_2)\| \le C \Big( \|u_1 - u_2\| + \|\alpha_1 - \alpha_2\| + \|\beta_1 - \beta_2\| \Big)$$

for all  $(u_1, \alpha_1, \beta_1), (u_2, \alpha_2, \beta_2) \in \mathbb{R}^n \times [0, \infty)^m \times [0, \infty)^m$  with  $||u_1||, ||u_2|| \leq M$ .

*Proof.* We proceed along the lines of [12, Theorem 2.6]: Suppose that a constant M > 0 is given, consider some  $(u_1, \alpha_1, \beta_1), (u_2, \alpha_2, \beta_2) \in \mathbb{R}^n \times [0, \infty)^m \times [0, \infty)^m$  with  $||u_1||, ||u_2|| \leq M$ , and denote the solutions of (V) associated with the triples  $(u_1, \alpha_1, \beta_1)$  and  $(u_2, \alpha_2, \beta_2)$  with  $y_1$  and  $y_2$ , respectively. Then, (3.1) yields that

$$\langle A(y_1), z \rangle + \sum_{k=1}^{m} \omega_k \Big( \alpha_{1,k} \| \cdot \|'(G_k y_1; G_k z) + \beta_{1,k} (\| \cdot \|^{1+\gamma})'(G_k y_1; G_k z) \Big) \ge \langle Bu_1, z \rangle$$

and

$$\langle A(y_2), z \rangle + \sum_{k=1}^m \omega_k \Big( \alpha_{2,k} \| \cdot \|'(G_k y_2; G_k z) + \beta_{2,k}(\| \cdot \|^{1+\gamma})'(G_k y_2; G_k z) \Big) \ge \langle B u_2, z \rangle$$

holds for all  $z \in \mathbb{R}^n$ . In particular, we may choose the vectors  $z = \pm(y_1 - y_2)$  and add the above two inequalities to obtain

$$\begin{aligned} (3.3) \\ \langle A(y_1) - A(y_2), y_1 - y_2 \rangle \\ &\leq \langle B(u_1 - u_2), y_1 - y_2 \rangle \\ &+ \sum_{k=1}^m \omega_k(\alpha_{1,k} - \alpha_{2,k}) \Big( \| \cdot \|'(G_k y_1; G_k(y_2 - y_1)) \Big) \\ &+ \sum_{k=1}^m \omega_k(\beta_{1,k} - \beta_{2,k}) \Big( (\| \cdot \|^{1+\gamma})'(G_k y_1; G_k(y_2 - y_1)) \Big) \\ &+ \sum_{k=1}^m \omega_k \alpha_{2,k} \Big( \| \cdot \|'(G_k y_1; G_k(y_2 - y_1)) + \| \cdot \|'(G_k y_2; G_k(y_1 - y_2)) \Big) \\ &+ \sum_{k=1}^m \omega_k \beta_{2,k} \Big( (\| \cdot \|^{1+\gamma})'(G_k y_1; G_k(y_2 - y_1)) + (\| \cdot \|^{1+\gamma})'(G_k y_2; G_k(y_1 - y_2)) \Big). \end{aligned}$$

Due to the convexity of the functions  $\|\cdot\|$  and  $\|\cdot\|^{1+\gamma}$  and the non-negativity of the vectors  $\alpha$ ,  $\beta$  and  $\omega$ , the last two sums on the right-hand side of (3.3) are non-positive and can be ignored (see [12, Lemma 2.3e)]. Further, we obtain from the Lipschitz continuity of  $\|\cdot\|$  and  $\|\cdot\|^{1+\gamma}$  on bounded subsets of  $\mathbb{R}^l$  and Proposition 3.1 that there exists a constant  $C = C(\omega, M, G_k) > 0$  with

$$\sum_{k=1}^{m} \omega_{k}(\alpha_{1,k} - \alpha_{2,k}) \Big( \| \cdot \|'(G_{k}y_{1}; G_{k}(y_{2} - y_{1})) \Big) \\ + \sum_{k=1}^{m} \omega_{k}(\beta_{1,k} - \beta_{2,k}) \Big( (\| \cdot \|^{1+\gamma})'(G_{k}y_{1}; G_{k}(y_{2} - y_{1})) \Big) \\ \leq C \left( \|\alpha_{1} - \alpha_{2}\| + \|\beta_{1} - \beta_{2}\| \right) \|y_{1} - y_{2}\|.$$

The claim now follows immediately from (3.3), the strong monotonicity of A and the inequality of Cauchy-Schwarz.  $\hfill \Box$ 

We are now in the position to prove the main result of this paper:

THEOREM 3.3 (Continuous Fréchet Differentiability of the Solution Map). The solution operator  $S : (u, \alpha, \beta) \mapsto y$  associated with the variational inequality (V) is continuously Fréchet differentiable as a function  $S : \mathbb{R}^n \times [0, \infty)^m \times (0, \infty)^m \to \mathbb{R}^n$ , i.e., there exists a continuous map S' which maps  $\mathbb{R}^n \times [0, \infty)^m \times (0, \infty)^m$  into the space  $L(\mathbb{R}^n \times \mathbb{R}^m \times \mathbb{R}^m, \mathbb{R}^n)$  of continuous and linear operators from  $\mathbb{R}^n \times \mathbb{R}^m \times \mathbb{R}^m$  to  $\mathbb{R}^n$  such that, for every  $w \in \mathbb{R}^n \times [0, \infty)^m \times (0, \infty)^m$ , we have

(3.4) 
$$\lim_{\substack{\|h\|\to 0,\\w+h\in\mathbb{R}^n\times[0,\infty)^m\times(0,\infty)^m}}\frac{\|S(w+h)-S(w)-S'(w)h\|}{\|h\|} = 0.$$

Moreover, for every triple  $(u, \alpha, \beta) \in \mathbb{R}^n \times [0, \infty)^m \times (0, \infty)^m$ , the Fréchet derivative  $S'(u, \alpha, \beta) \in L(\mathbb{R}^n \times \mathbb{R}^m \times \mathbb{R}^m, \mathbb{R}^n)$  is precisely the solution map  $(h_1, h_2, h_3) \mapsto \delta$  of the elliptic variational equality

$$\begin{cases}
\left\{ \begin{array}{l} \delta \in W(y), \\ \langle A'(y)\delta, z \rangle \\ + \sum_{k:G_k y \neq 0} \omega_k \left( \alpha_k \| \cdot \|''(G_k y)(G_k \delta, G_k z) + \beta_k (\| \cdot \|^{1+\gamma})''(G_k y)(G_k \delta, G_k z) \right) \\ = \langle Bh_1, z \rangle - \sum_{k:G_k y \neq 0} \omega_k \left( h_{2,k} \| \cdot \|'(G_k y)(G_k z) + h_{3,k} (\| \cdot \|^{1+\gamma})'(G_k y)(G_k z) \right) \\ \forall z \in W(y). \end{cases}$$

Here,  $y := S(u, \alpha, \beta)$  is the solution of (V) associated with the triple  $(u, \alpha, \beta)$ , A'(y) is the Fréchet derivative of A in y,  $\|\cdot\|'$  and  $(\|\cdot\|^{1+\gamma})'$  (respectively,  $\|\cdot\|''$  and  $(\|\cdot\|^{1+\gamma})'')$ are the first (respectively, second) Fréchet derivatives of the functions  $\|\cdot\|$  and  $\|\cdot\|^{1+\gamma}$ away from the origin, and W(y) is the subspace of  $\mathbb{R}^n$  defined by

(3.6) 
$$W(y) := \{ z \in \mathbb{R}^n \mid G_k z = 0 \text{ for all } k = 1, ..., m \text{ with } G_k y = 0 \}.$$

Note that, by direct calculation, we obtain that the variational equality (3.5) can also be written in the following, more explicit form:

$$\begin{split} \delta \in W(y), \\ \langle A'(y)\delta, z \rangle &+ \sum_{k \,:\, G_k y \neq 0} \omega_k \alpha_k \frac{\|G_k y\|^2 \left\langle G_k \delta, G_k z \right\rangle - \left\langle G_k y, G_k \delta \right\rangle \left\langle G_k y, G_k z \right\rangle}{\|G_k y\|^3} \\ &+ \sum_{k \,:\, G_k y \neq 0} \omega_k \beta_k (1+\gamma) \frac{\|G_k y\|^2 \left\langle G_k \delta, G_k z \right\rangle - \left\langle G_k y, G_k \delta \right\rangle \left\langle G_k y, G_k z \right\rangle}{\|G_k y\|^{3-\gamma}} \\ &+ \sum_{k \,:\, G_k y \neq 0} \omega_k \beta_k (\gamma^2 + \gamma) \frac{\left\langle G_k y, G_k \delta \right\rangle \left\langle G_k y, G_k z \right\rangle}{\|G_k y\|^{3-\gamma}} \\ &= \left\langle Bh_1, z \right\rangle - \sum_{k \,:\, G_k y \neq 0} \omega_k \left( h_{2,k} \frac{\left\langle G_k y, G_k z \right\rangle}{\|G_k y\|} + h_{3,k} (1+\gamma) \frac{\left\langle G_k y, G_k z \right\rangle}{\|G_k y\|^{1-\gamma}} \right) \\ &\quad \forall z \in W(y). \end{split}$$

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*Proof of Theorem 3.3.* To prove the different claims in Theorem 3.3, we proceed in several steps:

Step 1 (Gâteaux Differentiability): We begin by showing that the solution map S associated with (V) is Gâteaux differentiable everywhere in  $\mathbb{R}^n \times [0, \infty)^m \times (0, \infty)^m$ . The approach that we use in the following to establish the Gâteaux differentiability is fairly standard and relies heavily on the Lipschitz estimate (3.2) in Proposition 3.2. Compare, e.g., with [19, 29] in this context, and also with the more general theory for infinite-dimensional problems in [2, 10, 14].

Suppose that an arbitrary but fixed triple  $w := (u, \alpha, \beta) \in \mathbb{R}^n \times [0, \infty)^m \times (0, \infty)^m$ is given, and let  $h := (h_1, h_2, h_3)$  be a vector such that  $w + t_0 h \in \mathbb{R}^n \times [0, \infty)^m \times (0, \infty)^m$ holds for some  $t_0 > 0$ . Then, the convexity of the set  $\mathbb{R}^n \times [0, \infty)^m \times (0, \infty)^m$  implies that w + th is an element of  $\mathbb{R}^n \times [0, \infty)^m \times (0, \infty)^m$  for all  $t \in (0, t_0)$ , and we may define

$$\delta_t := \frac{S(w+th) - S(w)}{t} \in \mathbb{R}^n$$

for all  $t \in (0, t_0)$ . Due to the Lipschitz estimate (3.2), the difference quotients  $\delta_t$ remain bounded as t tends to zero. This implies in particular that, for every arbitrary but fixed sequence  $\{t_j\} \subset (0, t_0)$  with  $t_j \searrow 0$ , we can find a subsequence (still denoted by the same symbol) such that  $\delta_j := \delta_{t_j} \to \delta$  holds for some  $\delta \in \mathbb{R}^n$ . By defining y := S(w), by choosing test vectors of the form  $v := y + t_j z$ ,  $z \in \mathbb{R}^n$ , in the variational inequality for  $S(w + t_j h) = y + t_j \delta_j$ , by dividing by  $t_j^2$ , and by rearranging terms, we now obtain the following for all  $z \in \mathbb{R}^n$ :

$$\begin{cases} 3.7) \\ \left\langle \frac{A(y+t_{j}\delta_{j})-A(y)}{t_{j}}, z-\delta_{j} \right\rangle \\ + \sum_{k=1}^{m} \omega_{k}\alpha_{k} \frac{1}{t_{j}} \left( \frac{\|G_{k}y+t_{j}G_{k}z\|-\|G_{k}y\|}{t_{j}} - \|\cdot\|'(G_{k}y;G_{k}z) \right) \\ + \sum_{k=1}^{m} \omega_{k}\beta_{k} \frac{1}{t_{j}} \left( \frac{\|G_{k}y+t_{j}G_{k}z\|^{1+\gamma}-\|G_{k}y\|^{1+\gamma}}{t_{j}} - (\|\cdot\|^{1+\gamma})'(G_{k}y;G_{k}z) \right) \\ - \sum_{k=1}^{m} \omega_{k}\alpha_{k} \frac{1}{t_{j}} \left( \frac{\|G_{k}y+t_{j}G_{k}\delta_{j}\|-\|G_{k}y\|}{t_{j}} - \|\cdot\|'(G_{k}y;G_{k}\delta_{j}) \right) \\ - \sum_{k=1}^{m} \omega_{k}\beta_{k} \frac{1}{t_{j}} \left( \frac{\|G_{k}y+t_{j}G_{k}\delta_{j}\|^{1+\gamma}-\|G_{k}y\|^{1+\gamma}}{t_{j}} - (\|\cdot\|^{1+\gamma})'(G_{k}y;G_{k}\delta_{j}) \right) \\ + \frac{1}{t_{j}} \left( \langle A(y) - Bu, z \rangle + \sum_{k=1}^{m} \omega_{k} \left( \alpha_{k} \|\cdot\|'(G_{k}y;G_{k}z) + \beta_{k}(\|\cdot\|^{1+\gamma})'(G_{k}y;G_{k}z) \right) \right) \\ - \frac{1}{t_{j}} \left( \langle A(y) - Bu, \delta_{j} \rangle + \sum_{k=1}^{m} \omega_{k} \left( \alpha_{k} \|\cdot\|'(G_{k}y;G_{k}\delta_{j}) + \beta_{k}(\|\cdot\|^{1+\gamma})'(G_{k}y;G_{k}\delta_{j}) \right) \right) \\ \geq \langle Bh_{1}, z-\delta_{j} \rangle \\ + \sum_{k=1}^{m} \omega_{k}h_{2,k} \left( \frac{\|G_{k}y+t_{j}G_{k}\delta_{j}\|-\|G_{k}y+t_{j}G_{k}z\|}{t_{j}} \right) \\ + \sum_{k=1}^{m} \omega_{k}h_{3,k} \left( \frac{\|G_{k}y+t_{j}G_{k}\delta_{j}\|^{1+\gamma}-\|G_{k}y+t_{j}G_{k}z\|^{1+\gamma}}{t_{j}} \right). \end{cases}$$

Note that we have added several terms here (e.g., the norms  $||G_ky||$ ), so that the expressions on the left-hand side of (3.7) take the form of classical difference quotients. An important observation at this point is that all of the terms in the large round brackets on the left-hand side of (3.7) are non-negative (the second-order difference quotients of the functions  $|| \cdot ||$  and  $|| \cdot ||^{1+\gamma}$  due to convexity and the terms in the last two lines of the left-hand side of (3.7) due to (3.1)). This allows us to deduce the following from (3.7) when we choose z to be zero: (3.8)

$$0 \leq \sum_{k:G_{k}y=0} \omega_{k}\beta_{k} \frac{\|G_{k}\delta_{j}\|^{1+\gamma}}{t_{j}^{1-\gamma}}$$

$$= \sum_{k:G_{k}y=0} \omega_{k}\beta_{k} \frac{1}{t_{j}} \left( \frac{\|G_{k}y+t_{j}G_{k}\delta_{j}\|^{1+\gamma}-\|G_{k}y\|^{1+\gamma}}{t_{j}} - (\|\cdot\|^{1+\gamma})'(G_{k}y;G_{k}\delta_{j}) \right)$$

$$\leq \left\langle Bh_{1} - \frac{A(y+t_{j}\delta_{j}) - A(y)}{t_{j}}, \delta_{j} \right\rangle$$

$$- \sum_{k=1}^{m} \omega_{k}h_{2,k} \left( \frac{\|G_{k}y+t_{j}G_{k}\delta_{j}\| - \|G_{k}y\|}{t_{j}} \right)$$

$$- \sum_{k=1}^{m} \omega_{k}h_{3,k} \left( \frac{\|G_{k}y+t_{j}G_{k}\delta_{j}\|^{1+\gamma} - \|G_{k}y\|^{1+\gamma}}{t_{j}} \right).$$

Since the right-hand side of (3.8) remains bounded for  $t_j \searrow 0$ , since  $\gamma \in (0, 1)$  and since  $\omega_k \beta_k > 0$  for all k, the above implies that the limit  $\delta$  of the difference quotients  $\delta_j$  is contained in the set  $W(y) = \{z \in \mathbb{R}^n \mid G_k z = 0 \text{ for all } k \text{ with } G_k y = 0\}$ . From (3.7), the fact that (3.1) holds with equality for all  $z \in W(y)$ , and again the information about the signs of the terms in (3.7), we now obtain that  $\delta_j$  satisfies (3.9)

$$\begin{split} \left\langle \frac{\dot{A}(y+t_{j}\delta_{j})-A(y)}{t_{j}}, z-\delta_{j} \right\rangle \\ &+ \sum_{k:G_{k}y\neq0} \omega_{k}\alpha_{k} \frac{1}{t_{j}} \left( \frac{\|G_{k}y+t_{j}G_{k}z\| - \|G_{k}y\|}{t_{j}} - \|\cdot\|'(G_{k}y)(G_{k}z) \right) \\ &+ \sum_{k:G_{k}y\neq0} \omega_{k}\beta_{k} \frac{1}{t_{j}} \left( \frac{\|G_{k}y+t_{j}G_{k}z\|^{1+\gamma} - \|G_{k}y\|^{1+\gamma}}{t_{j}} - (\|\cdot\|^{1+\gamma})'(G_{k}y)(G_{k}z) \right) \\ &- \sum_{k:G_{k}y\neq0} \omega_{k}\alpha_{k} \frac{1}{t_{j}} \left( \frac{\|G_{k}y+t_{j}G_{k}\delta_{j}\| - \|G_{k}y\|}{t_{j}} - \|\cdot\|'(G_{k}y)(G_{k}\delta_{j}) \right) \\ &- \sum_{k:G_{k}y\neq0} \omega_{k}\beta_{k} \frac{1}{t_{j}} \left( \frac{\|G_{k}y+t_{j}G_{k}\delta_{j}\|^{1+\gamma} - \|G_{k}y\|^{1+\gamma}}{t_{j}} - (\|\cdot\|^{1+\gamma})'(G_{k}y)(G_{k}\delta_{j}) \right) \\ &\geq \langle Bh_{1}, z-\delta_{j} \rangle \\ &+ \sum_{k=1}^{m} \omega_{k}h_{2,k} \left( \frac{\|G_{k}y+t_{j}G_{k}\delta_{j}\| - \|G_{k}y\|}{t_{j}} - \frac{\|G_{k}y+t_{j}G_{k}z\| - \|G_{k}y\|}{t_{j}} \right) \\ &+ \sum_{k=1}^{m} \omega_{k}h_{3,k} \left( \frac{\|G_{k}y+t_{j}G_{k}\delta_{j}\|^{1+\gamma} - \|G_{k}y\|^{1+\gamma}}{t_{j}} - \frac{\|G_{k}y+t_{j}G_{k}z\|^{1+\gamma} - \|G_{k}y\|^{1+\gamma}}{t_{j}} \right) \end{split}$$

for all  $z \in W(y)$ . Note that all of the expressions in (3.9) are well-behaved for  $j \to \infty$  (since the Euclidean norm  $\|\cdot\|$  is smooth away from the origin and Hadamard

directionally differentiable everywhere, and since A is Fréchet). We may thus pass to the limit to arrive at the following variational inequality of the second kind: (3.10)

$$\begin{split} \langle A'(y)\delta - Bh_1, z - \delta \rangle \\ &+ \frac{1}{2} \sum_{k:G_k y \neq 0} \omega_k \Big( \alpha_k \| \cdot \|''(G_k y)(G_k z, G_k z) + \beta_k (\| \cdot \|^{1+\gamma})''(G_k y)(G_k z, G_k z) \Big) \\ &- \frac{1}{2} \sum_{k:G_k y \neq 0} \omega_k \Big( \alpha_k \| \cdot \|''(G_k y)(G_k \delta, G_k \delta) + \beta_k (\| \cdot \|^{1+\gamma})''(G_k y)(G_k \delta, G_k \delta) \Big) \\ &\geq - \sum_{k:G_k y \neq 0} \omega_k \Big( h_{2,k} \frac{\langle G_k y, G_k (z - \delta) \rangle}{\|G_k y\|} + h_{3,k} (1+\gamma) \frac{\langle G_k y, G_k (z - \delta) \rangle}{\|G_k y\|^{1-\gamma}} \Big) \\ &\quad \forall z \in W(y). \end{split}$$

Since the Fréchet derivative  $A'(y) : \mathbb{R}^n \to \mathbb{R}^n$  inherits the strong monotonicity of the original operator A (see [10, Lemma 1.2.3]), the problem (3.10) can have at most one solution  $\delta \in W(y)$  (cf. step 3 in the proof of [10, Theorem 1.2.2]), and we may deduce that the limit  $\delta$  of the difference quotients  $\delta_j$  is independent of the choice of the (sub)sequence  $\{t_j\} \subset (0, t_0)$  that we started with. The latter implies, in combination with classical contradiction arguments, that the whole family of difference quotients  $\{\delta_t\}$  converges to the unique solution  $\delta \in W(y)$  of (3.10) for  $t \searrow 0$ , and that the solution operator S associated with (V) is directionally differentiable in the point win every direction h with  $w + t_0 h \in \mathbb{R}^n \times [0, \infty)^m \times (0, \infty)^m$  for some  $t_0 > 0$ . By choosing test vectors of the form  $\delta + sz$ ,  $z \in \mathbb{R}^n$ , s > 0, in (3.10), by dividing by s, by passing to the limit  $s \searrow 0$ , and by exploiting that W(y) is a subspace, we obtain further that (3.10) can be rewritten as (3.5). Since (3.5) has a linear and continuous solution operator  $(h_1, h_2, h_3) \mapsto \delta$ , it now follows immediately that the map S is Gâteaux differentiable in w and that the derivative  $S'(w) \in L(\mathbb{R}^n \times \mathbb{R}^m \times \mathbb{R}^m, \mathbb{R}^n)$  is characterized by (3.5). This completes the first step of the proof.

Step 2 (Fréchet Differentiability): The Fréchet differentiability of the solution map S on  $\mathbb{R}^n \times [0, \infty)^m \times (0, \infty)^m$  follows immediately from the Gâteaux differentiability of S, the Lipschitz estimate (3.2) and standard arguments. We include the proof for the convenience of the reader: Suppose that there exists a  $w \in \mathbb{R}^n \times [0, \infty)^m \times (0, \infty)^m$  such that S is not Fréchet differentiable in w in the sense of (3.4). Then, there exist an  $\varepsilon > 0$  and sequences  $\{h_j\} \subset \mathbb{R}^n \times \mathbb{R}^m \times \mathbb{R}^m$ ,  $\{t_j\} \subset (0, \infty)$  such that  $t_j \searrow 0$  for  $j \to \infty$ ,  $\|h_j\| = 1$  for all j,  $w + t_j h_j \in \mathbb{R}^n \times [0, \infty)^m \times (0, \infty)^m$  for all j, and

$$||S(w+t_jh_j) - S(w) - t_j S'(w)h_j|| \ge \varepsilon t_j \qquad \forall j$$

Since  $||h_j|| = 1$ , we may assume w.l.o.g. that  $h_j \to h$  holds for some  $h \in \mathbb{R}^n \times \mathbb{R}^m \times \mathbb{R}^m$ , and from the properties of the sequence  $\{h_j\}$  (or the signs of the components of  $h_j$ , to be more precise), it follows straightforwardly that there has to be an s > 0 with  $w + sh \in \mathbb{R}^n \times [0, \infty)^m \times (0, \infty)^m$ . From the local Lipschitz continuity of S, we may now deduce that

$$\varepsilon \leq \frac{\|S(w+t_jh_j) - S(w) - t_jS'(w)h_j\|}{t_j} = \frac{\|S(w+t_jh) - S(w) - t_jS'(w)h\|}{t_j} + o(1),$$

where the Landau symbol refers to the limit  $j \to \infty$ . This is a contradiction with the Gâteaux differentiability that we have established in the first part of the proof. Thus, S is Fréchet differentiable and the second step of the proof is complete.

Step 3 (Continuity of the Fréchet Derivative): It remains to prove that the map  $S': \mathbb{R}^n \times [0,\infty)^m \times (0,\infty)^m \to L(\mathbb{R}^n \times \mathbb{R}^m \times \mathbb{R}^m, \mathbb{R}^n)$  is continuous. To this end, we consider an arbitrary but fixed sequence  $\{w_j\} \subset \mathbb{R}^n \times [0,\infty)^m \times (0,\infty)^m$  which satisfies  $w_j = (u_j, \alpha_j, \beta_j) \to w = (u, \alpha, \beta)$  for some  $w \in \mathbb{R}^n \times [0,\infty)^m \times (0,\infty)^m$ . Note that, to prove the continuity of S', it suffices to show that  $S'(w_j)h \to S'(w)h$  holds for all  $h \in \mathbb{R}^n \times \mathbb{R}^m \times \mathbb{R}^m$  (since this convergence already implies  $S'(w_j) \to S(w)$  in the operator norm). So let us assume that an  $h = (h_1, h_2, h_3) \in \mathbb{R}^n \times \mathbb{R}^m \times \mathbb{R}^m$  is given. Then, (3.5) yields that the vectors  $\eta_j := S'(w_j)h$  satisfy

$$\eta_j \in W(y_j) = \{ z \in \mathbb{R}^n \mid G_k z = 0 \text{ for all } k = 1, ..., m \text{ with } G_k y_j = 0 \}$$

and

$$\begin{aligned} A'(y_{j})\eta_{j},\eta_{j}\rangle \\ &+ \sum_{k:G_{k}y_{j}\neq0} \omega_{k}\alpha_{j,k} \frac{\|G_{k}y_{j}\|^{2}\|G_{k}\eta_{j}\|^{2} - \langle G_{k}y_{j},G_{k}\eta_{j}\rangle^{2}}{\|G_{k}y_{j}\|^{3}} \\ &+ \sum_{k:G_{k}y_{j}\neq0} \omega_{k}\beta_{j,k}(1+\gamma) \frac{\|G_{k}y_{j}\|^{2}\|G_{k}\eta_{j}\|^{2} - (1-\gamma)\langle G_{k}y_{j},G_{k}\eta_{j}\rangle^{2}}{\|G_{k}y_{j}\|^{3-\gamma}} \\ &= \langle Bh_{1},\eta_{j}\rangle - \sum_{k:G_{k}y_{j}\neq0} \omega_{k} \Big(h_{2,k} \frac{\langle G_{k}y_{j},G_{k}\eta_{j}\rangle}{\|G_{k}y_{j}\|} + h_{3,k}(1+\gamma) \frac{\langle G_{k}y_{j},G_{k}\eta_{j}\rangle}{\|G_{k}y_{j}\|^{1-\gamma}} \Big) \end{aligned}$$

Here,  $y_j$  is short for  $S(w_j)$ . From the strong monotonicity of  $A'(y_j)$  (which is uniform in j by our assumptions and [10, Lemma 1.2.3]) and the inequalities of Cauchy-Schwarz and Young, we may now deduce that there exist constants c, C > 0 independent of jwith

(3.11) 
$$c\|\eta_j\|^2 + \sum_{k:G_k y_j \neq 0} \omega_k \beta_{j,k} (\gamma^2 + \gamma) \frac{\|G_k \eta_j\|^2}{\|G_k y_j\|^{1-\gamma}} \le C.$$

The above implies that the sequence  $\{\eta_j\}$  is bounded and that we may pass over to a subsequence (still denoted by the same symbol) with  $\eta_j \to \eta$  for some  $\eta$ . We claim that this  $\eta$  satisfies  $\eta \in W(y)$ , where y := S(w) is the solution associated with the limit point w. To see this, we consider an arbitrary but fixed  $k \in \{1, ..., m\}$  with  $G_k y = 0$  and distinguish between two cases: If we can find a subsequence  $j_i$  such that  $G_k y_{j_i} = 0$  holds for all i, then we trivially have  $G_k \eta_{j_i} = 0$  for all i (since  $\eta_{j_i} \in W(y_{j_i})$ ), and we immediately obtain from the convergence  $\eta_{j_i} \to \eta$  that  $G_k \eta = 0$ . If, on the other hand, we can find a subsequence  $j_i$  such that  $G_k y_{j_i} \neq 0$  holds for all i, then (3.11) yields

$$0 \le \omega_k \beta_{j_i,k} (\gamma^2 + \gamma) \| G_k \eta_{j_i} \|^2 \le C \| G_k y_{j_i} \|^{1-\gamma}$$

and we may use the convergences  $y_{j_i} \to y$  and  $\beta_{j_i} \to \beta \in (0, \infty)^m$  to conclude that  $G_k \eta = 0$ . This shows that  $G_k \eta = 0$  holds for all k with  $G_k y = 0$  and that  $\eta$  is indeed an element of W(y). Suppose now that j is so large that  $G_k y_j \neq 0$  holds for all  $k \in \{1, ..., m\}$  with  $G_k y \neq 0$  (this is the case for all large enough j due to the convergence  $y_j \to y$ ). Then, it clearly holds  $W(y) \subset W(y_j)$ , and we may deduce the

following from the variational equality (3.5) for  $\eta_j$ :

$$\begin{split} \langle A'(y_j)\eta_j, z \rangle \\ &+ \sum_{k:\,G_k y \neq 0} \omega_k \alpha_{j,k} \frac{\|G_k y_j\|^2 \langle G_k \eta_j, G_k z \rangle - \langle G_k y_j, G_k \eta_j \rangle \langle G_k y_j, G_k z \rangle}{\|G_k y_j\|^3} \\ &+ \sum_{k:\,G_k y \neq 0} \omega_k \beta_{j,k} (1+\gamma) \frac{\|G_k y_j\|^2 \langle G_k \eta_j, G_k z \rangle - \langle G_k y_j, G_k \eta_j \rangle \langle G_k y_j, G_k z \rangle}{\|G_k y_j\|^{3-\gamma}} \\ &+ \sum_{k:\,G_k y \neq 0} \omega_k \beta_{j,k} (\gamma^2 + \gamma) \frac{\langle G_k y_j, G_k \eta_j \rangle \langle G_k y_j, G_k z \rangle}{\|G_k y_j\|^{3-\gamma}} \\ &= \langle Bh_1, z \rangle - \sum_{k:\,G_k y \neq 0} \omega_k \left( h_{2,k} \frac{\langle G_k y_j, G_k z \rangle}{\|G_k y_j\|} + h_{3,k} (1+\gamma) \frac{\langle G_k y_j, G_k z \rangle}{\|G_k y_j\|^{1-\gamma}} \right) \\ &\quad \forall z \in W(y). \end{split}$$

If we pass to the limit  $j \to \infty$  in the above, then it follows that  $\eta$  solves the variational problem (3.5) which characterizes S'(w)h. This shows that  $\eta = S'(w)h$  has to hold and that  $S'(w_j)h$  converges to S'(w)h for  $j \to \infty$ . Using the same arguments as in the first part of the proof, we obtain that this convergence also holds for the whole original sequence  $S'(w_j)h$  and not just for the subsequence that we have chosen after (3.11). This proves the continuity of S' and completes the proof.

Some remarks are in order regarding Theorem 3.3:

Remark 3.4.

. . . . .

- 1. It seems to be a common believe that minimization problems and elliptic variational inequalities which involve non-differentiable terms necessarily also have non-differentiable solution operators. Theorem 3.3 shows that there is, in fact, no such automatism, and that it is perfectly possible that the solution map of a non-smooth problem is continuously Fréchet differentiable. In the fields of bilevel optimization and optimal control, this observation is, of course, very valuable.
- 2. We would like to point out that the solution map S associated with (V) is typically not Fréchet differentiable in points  $(u, \alpha, \beta)$  with  $\beta_k = 0$  for some k. Theorem 3.3 thus does not hold anymore in general when we replace the set  $\mathbb{R}^n \times [0, \infty)^m \times (0, \infty)^m$  with  $\mathbb{R}^n \times [0, \infty)^m \times [0, \infty)^m$ . Similarly, we cannot expect Fréchet differentiability anymore when the exponent  $\gamma$  is equal to zero or one. The fact that S is not Fréchet differentiable for  $\gamma = 0$  and  $\gamma = 1$ but for all  $\gamma$  between these values is quite counterintuitive. Note that, in all of the above cases, the solution operator is still Hadamard directionally differentiable in the sense of [5, Definition 2.45] as one may easily check using the same arguments as in the first step of the proof of Theorem 3.3.
- 3. What we observe in Theorem 3.3 can be interpreted as a non-standard regularization effect. Consider, for instance, the simple model problem

(3.12) 
$$\begin{cases} \min \|y - y_D\|^2 + \frac{\mu}{2} \left(\|u\|^2 + \alpha^2\right) \\ \text{s.t. } y \in \mathbb{R}^n, \ u \in \mathbb{R}^n, \ \alpha \in [0, \infty), \\ y = \operatorname*{argmin}_{v \in \mathbb{R}^n} \frac{1}{2} \|v - u\|^2 + \alpha \|v\|_1, \end{cases}$$

where  $y_D \in \mathbb{R}^n$  and  $\mu > 0$  are given, and where  $\|\cdot\|_1$  denotes the 1-norm on the Euclidean space. Then, it is easy to check that the solution operator  $S : \mathbb{R}^n \times [0, \infty) \to \mathbb{R}^n$ ,  $(u, \alpha) \mapsto y$ , associated with the inner minimization problem in (3.12) is non-smooth. In fact, in the special case n = 1, we can derive the following closed formula for the solution map:

(3.13) 
$$S(u,\alpha) = \begin{cases} u+\alpha & \text{if } u \leq -\alpha \\ 0 & \text{if } u \in (-\alpha,\alpha) \\ u-\alpha & \text{if } u \geq \alpha \end{cases}$$

Suppose now that we modify (3.12) by adding a term of the form  $\varepsilon ||v||_p^p$  for some  $p \in (1,2)$  in the lower-level problem, where  $\varepsilon > 0$  is an arbitrary but fixed small number and where  $|| \cdot ||_p$  denotes the *p*-norm on  $\mathbb{R}^n$ . Then, the resulting bilevel minimization problem

(3.14) 
$$\begin{cases} \min \|y - y_D\|^2 + \frac{\mu}{2} \left(\|u\|^2 + \alpha^2\right) \\ \text{s.t.} \quad y \in \mathbb{R}^n, \ u \in \mathbb{R}^n, \ \alpha \in [0, \infty), \\ y = \operatorname*{argmin}_{v \in \mathbb{R}^n} \frac{1}{2} \|v - u\|^2 + \alpha \|v\|_1 + \varepsilon \|v\|_p^p \end{cases}$$

can also be written in the form (P) (cf. the second example in Section 2), and we obtain from Theorem 3.3 that the solution operator  $S_{\varepsilon} : \mathbb{R}^n \times [0, \infty) \to \mathbb{R}^n$ ,  $(u, \alpha) \mapsto y$ , associated with the lower level of (3.14) is continuously Fréchet differentiable. By adding the term  $\varepsilon \| \cdot \|_p^p$ , we have thus indeed regularized the original problem (3.12). What is appealing about the above method of regularization is that it is "minimally invasive". It produces an approximate problem whose reduced objective function possesses  $C^1$ -regularity (and which is thus amenable to gradient-based solution algorithms, see Section 4) while preserving the non-smooth features and, e.g., the sparsity promoting nature on the lower level. Note that the addition of the term  $\varepsilon \| \cdot \|_{p}^{p}$  in particular does not change the subdifferential at zero of the objective function of the inner problem in (3.12). We would like to emphasize at this point that the lowerlevel problems in (3.12) and (3.14) can be solved easily with various standard algorithms (e.g., semi-smooth Newton, subgradient or bundle methods). The major difficulty in (3.12) is handling the non-smoothness of the solution map  $S:(u,\alpha)\mapsto y$  on the upper level. In view of these facts, the regularization effect observed above is the best that we can hope for: By adding the term  $\varepsilon \parallel \cdot \parallel_p^p$ , we regularize the solution operator of the inner problem in (3.12) without regularizing the non-differentiable terms in the inner problem. This removes the non-smoothness where it is problematic (in the solution map) while preserving it where it can be handled (in the lower-level problem). At least to the author's best knowledge, similar effects have not been documented so far in the literature (where primarily Huber-type regularizations are used which do not preserve sparsity promoting effects, see [8, 15, 20, 28, 36]).

4. In the context of the general sensitivity analysis for elliptic variational inequalities of the first and the second kind developed in [2, 10, 39], the differentiability result in Theorem 3.3 can be explained as follows: The singular curvature properties of the terms  $||G_k(\cdot)||^{1+\gamma}$  at the origin enforce that the second subderivative of the non-smooth functional in (V) is generated by a symmetric bilinear form defined on a subspace of  $\mathbb{R}^n$  (namely, the space W(y) in (3.6)). This, in combination with the second-order epi-differentiability of the involved terms, yields the Fréchet differentiability of the solution operator to (V). For details on this topic and the underlying theory, we refer to [10, Chapters 1 and 4, Theorem 1.4.1, Corollary 1.4.4].

- 5. The regularization effect in Theorem 3.3 can also be exploited in the infinitedimensional setting (see, for instance, [10, Section 4.3.3] for a simple example). However, in infinite dimensions, one typically requires additional Lipschitz continuity/compactness properties to establish the directional differentiability of the solution map S and the analysis becomes much more involved (cf. the approach in [12] where superposition operators are considered). In particular, it does not seem to be possible to derive a "general purpose" result analogous to Theorem 3.3 for elliptic variational inequalities in arbitrary Hilbert spaces.
- 6. Results analogous to Theorem 3.3 can also be obtained for problems which involve non-smooth functions whose properties are similar to those of the Euclidean norm (e.g., the maximum function  $\max(0, \cdot)$ ).
- 7. It should be noted that the variational problem (3.5) that characterizes the operators S'(w) arises from the original variational inequality (V) by termwise differentiation (where, at the origin, the missing second derivative of the Euclidean norm is replaced with the conditions in (3.6)). Compare also with the alternative formulation (3.10) in this context. An analogous behavior can be observed for smooth problems, cf., e.g., the results in [5].

4. Consequences for the Applicability of Gradient-Based Algorithms. The consequences that Theorem 3.3 has for the analysis and the numerical solution of the bilevel optimization and optimal control problems in Sections 1 and 2 are obvious: Since the solution operator  $S: (u, \alpha, \beta) \mapsto y$  associated with the elliptic variational inequality (V) is continuously Fréchet differentiable on  $\mathbb{R}^n \times [0,\infty)^m \times (0,\infty)^m$ , we can tackle every problem of the type (P) that satisfies the conditions in Assumption 1.1 with standard gradient-based algorithms. Depending on the precise nature of the problem at hand, possible choices could be, for instance, trust-region methods, see [11, 16, 34], (projected) gradient methods, see [4, 23, 27], or non-linear conjugated gradient methods, see [23, 34, 37]. For a tangible example of a solution algorithm, we refer to Section 5. Note that our standing assumption  $U_{ad} \subset \mathbb{R}^n \times [0,\infty)^m \times (0,\infty)^m$ is indispensable at this point since Theorem 3.3 does not yield any information about S on the cone  $\{(u, \alpha, \beta) \in \mathbb{R}^n \times [0, \infty)^m \times [0, \infty)^m \mid \beta_k = 0 \text{ for some } k\}.$  (The author suspects that it is still possible to identify subgradients on this critical set by exploiting (3.1), cf. the analysis in [13, 38].) Further, it should be noted that all of the above-mentioned algorithms require evaluations of the derivative of the reduced objective function  $F(u, \alpha, \beta) := J(S(u, \alpha, \beta), u, \alpha, \beta)$  associated with the problem (P). To calculate the gradients of F efficiently, we can use an adjoint calculus as the following theorem shows:

THEOREM 4.1 (Calculation of Gradients). In the situation of Assumption 1.1, the Fréchet derivative  $F'(u, \alpha, \beta) \in \mathbb{R}^n \times \mathbb{R}^m \times \mathbb{R}^m$  of the reduced objective function  $F(u, \alpha, \beta) := J(S(u, \alpha, \beta), u, \alpha, \beta)$  in a point  $(u, \alpha, \beta) \in \mathbb{R}^n \times [0, \infty)^m \times (0, \infty)^m$  is given by

$$F'(u,\alpha,\beta) = \left( (\partial_u J)(y,u,\alpha,\beta) + B^* p_1, (\partial_\alpha J)(y,u,\alpha,\beta) + p_2, (\partial_\beta J)(y,u,\alpha,\beta) + p_3 \right)$$

Here, y is short for  $S(u, \alpha, \beta)$ ,  $p_1 = p_1(u, \alpha, \beta) \in \mathbb{R}^n$  is the unique solution of (4.1)

$$\begin{cases} p_1 \in W(y), \\ \langle A'(y)^* p_1, z \rangle \\ + \sum_{k: G_k y \neq 0} \omega_k \Big( \alpha_k \| \cdot \|''(G_k y)(G_k p_1, G_k z) + \beta_k (\| \cdot \|^{1+\gamma})''(G_k y)(G_k p_1, G_k z) \Big) \\ = \langle (\partial_y J)(y, u, \alpha, \beta), z \rangle & \forall z \in W(y), \end{cases}$$

the vectors  $p_2, p_3 \in \mathbb{R}^m$  are defined by

$$(p_2)_k := \begin{cases} -\omega_k \frac{\langle G_k y, G_k p_1 \rangle}{\|G_k y\|} & \text{if } G_k y \neq 0\\ 0 & \text{else} \end{cases}, \qquad k = 1, ..., m,$$

and

$$(p_3)_k := \begin{cases} -(1+\gamma)\omega_k \frac{\langle G_k y, G_k p_1 \rangle}{\|G_k y\|^{1-\gamma}} & \text{if } G_k y \neq 0\\ 0 & \text{else,} \end{cases}, \qquad k = 1, ..., m,$$

W(y) denotes the space in (3.6),  $B^*$  and  $A'(y)^*$  are the adjoints of B and A'(y)(w.r.t. the Euclidean scalar product), and  $\partial_y J$ ,  $\partial_u J$ ,  $\partial_\alpha J$  and  $\partial_\beta J$  denote the partial derivatives of the function J w.r.t. the first, the second, the third and the fourth argument, respectively.

*Proof.* From the chain rule, see [5, Proposition 2.47], it follows straightforwardly that, for every point  $(u, \alpha, \beta) \in \mathbb{R}^n \times [0, \infty)^m \times (0, \infty)^m$  and every  $h = (h_1, h_2, h_3) \in \mathbb{R}^n \times \mathbb{R}^m \times \mathbb{R}^m$ , we have

$$\langle F'(u,\alpha,\beta),h\rangle = \langle (\partial_y J)(y,u,\alpha,\beta),S'(u,\alpha,\beta)h\rangle + \langle (\partial_u J)(y,u,\alpha,\beta),h_1\rangle + \langle (\partial_\alpha J)(y,u,\alpha,\beta),h_2\rangle + \langle (\partial_\beta J)(y,u,\alpha,\beta),h_3\rangle.$$

Further, we obtain from the variational equality (3.5) for  $\delta := S'(u, \alpha, \beta)h \in W(y)$ and the definitions of the vectors  $p_1, p_2$ , and  $p_3$  that

$$\begin{aligned} \langle (\partial_y J)(y, u, \alpha, \beta), \delta \rangle \\ &= \langle A'(y)^* p_1, \delta \rangle \\ &+ \sum_{k:G_k y \neq 0} \omega_k \Big( \alpha_k \| \cdot \|''(G_k y)(G_k p_1, G_k \delta) + \beta_k (\| \cdot \|^{1+\gamma})''(G_k y)(G_k p_1, G_k \delta) \Big) \\ &= \langle Bh_1, p_1 \rangle - \sum_{k:G_k y \neq 0} \omega_k \Big( h_{2,k} \| \cdot \|'(G_k y)(G_k p_1) + h_{3,k} (\| \cdot \|^{1+\gamma})'(G_k y)(G_k p_1) \Big) \\ &= \langle B^* p_1, h_1 \rangle + \langle p_2, h_2 \rangle + \langle p_3, h_3 \rangle \,. \end{aligned}$$

The claim now follows immediately.

Note that every evaluation of the derivative F' requires the solution of the nonsmooth elliptic variational inequality (V) (since we need y). This, however, is not a major problem. As we have already mentioned in Remark 3.4, the inequality (V) is comparatively well-behaved and can be tackled with various standard algorithms (especially when it can be identified with a minimization problem of the type (1.1)). Compare also with the approach in Section 5 in this context.

5. An Example of a Solution Algorithm and a Numerical Experiment. In what follows, we demonstrate by means of a tangible example that the results in Theorems 3.3 and 4.1 indeed allow to solve problems of the type (P) with standard gradient-based algorithms. As a model problem, we consider a special instance of the optimal control problem for Casson fluids that we have derived in Section 2.1, namely, (5.1)

$$\begin{cases} \min \frac{1}{2} \langle B(y - y_D), y - y_D \rangle + \frac{\mu}{2} \left( \langle Bu, u \rangle + \alpha^2 \right) \\ \text{s.t.} \quad y, u \in \mathbb{R}^n, \ \alpha \in [\kappa, \infty), \\ y = \underset{v \in \mathbb{R}^n}{\operatorname{argmin}} \frac{1}{2} \langle Av, v \rangle + \sum_{k=1}^m |T_k| \left( \alpha |G_k v| + \frac{4}{3} \alpha^{1/2} |G_k v|^{3/2} \right) - \langle Bu, v \rangle. \end{cases}$$

Here, we have chosen the dimension d to be one (so that the Euclidean norms in (2.1) are just absolute value functions),  $\kappa \in (0, \infty)$  is a given constant (a lower bound for the Oldroyd number  $\alpha$ ) and the quantities A, B etc. are defined as in Section 2.1. To solve the problem (5.1), we will employ a standard gradient projection method in the spirit of [4, 23, 27], see Algorithm 5.4 below. We would like to emphasize that the subsequent analysis should be understood as a feasibility study. With Theorems 3.3 and 4.1 at our disposal, we could also consider more complicated problems and more sophisticated algorithms at this point (e.g., non-linear conjugated gradient or trust-region methods). To avoid overloading this paper, we leave a detailed discussion of the various possible applications of Theorems 3.3 and 4.1 (e.g., in the fields of parameter learning and identification, see Section 2.2) for future research.

Before we state the algorithm that we use for the solution of the optimization problem (5.1), we prove some auxiliary results:

LEMMA 5.1 (Multiplier System for the Lower-Level Problem in (5.1)). A vector  $y \in \mathbb{R}^n$  solves the lower-level problem in (5.1) for a given tuple  $(u, \alpha) \in \mathbb{R}^n \times (0, \infty)$  if and only if there exist multipliers  $\lambda_1, ..., \lambda_m, \eta_1, ..., \eta_m \in \mathbb{R}$  such that

(5.2) 
$$\begin{cases} Ay + \sum_{k=1}^{m} |T_k| \left( \alpha G_k^* \lambda_k + 2\alpha^{1/2} G_k^* \eta_k \right) - Bu = 0, \\ \max \left( \lambda_k^2 - 1, |G_k y| - (G_k y) \lambda_k \right) = 0, \quad k = 1, ..., m, \\ \max \left( \eta_k^2 - |G_k y|, |G_k y|^{3/2} - (G_k y) \eta_k \right) = 0, \quad k = 1, ..., m. \end{cases}$$

*Proof.* From standard calculus rules for the convex subdifferential (see, e.g., [22]), we obtain that a vector  $y \in \mathbb{R}^n$  solves the lower-level problem in (5.1) if and only if there exist  $\lambda_1, ..., \lambda_m, \eta_1, ..., \eta_m \in \mathbb{R}$  with

(5.3) 
$$\begin{cases} Ay + \sum_{k=1}^{m} |T_k| \left( \alpha G_k^* \lambda_k + 2\alpha^{1/2} G_k^* \eta_k \right) - Bu = 0, \\ \lambda_k \in \partial |\cdot| (G_k y), \qquad \forall k = 1, ..., m, \\ \eta_k \in \partial \left( \frac{2}{3} |\cdot|^{3/2} \right) (G_k y), \qquad \forall k = 1, ..., m. \end{cases}$$

If we plug in explicit formulas for the convex subdifferentials of the functions  $|\cdot|$  and  $|\cdot|^{3/2}$  in the above, then it follows straightforwardly that y and the multipliers  $\lambda_k$ 

and  $\eta_k$  satisfy the system (5.2). This proves the first implication. If, conversely, we start with the system (5.2), then the conditions on  $\lambda_k$  yield  $|\lambda_k| \leq 1$  and

$$0 \ge |G_k y| - (G_k y)\lambda_k \ge |G_k y||\lambda_k| - (G_k y)\lambda_k \ge 0$$

for all k = 1, ..., m. The above entails

$$|\lambda_k| \le 1$$
 for all  $k$  and  $\lambda_k = \operatorname{sgn}(G_k y)$  for all  $k$  with  $G_k y \ne 0$ 

which is equivalent to  $\lambda_k \in \partial |\cdot|(G_k y)$  for all k. For the multipliers  $\eta_k$ , we obtain along the same lines that  $|\eta_k| \leq |G_k y|^{1/2}$  and

$$0 \ge |G_k y|^{3/2} - (G_k y)\eta_k \ge |G_k y||\eta_k| - (G_k y)\eta_k \ge 0$$

holds for all k = 1, ..., m. This yields

$$\eta_k = \begin{cases} 0 & \text{for all } k \text{ with } G_k y = 0\\ \frac{G_k y}{|G_k y|^{1/2}} & \text{for all } k \text{ with } G_k y \neq 0 \end{cases}$$

and, as a consequence,  $\eta_k \in \partial\left(\frac{2}{3}|\cdot|^{3/2}\right)(G_k y)$  for all k = 1, ..., m. This shows that (5.2) is equivalent to (5.3) and completes the proof.

Note that the system (5.2) is amenable to numerical solution by a semi-smooth Newton method. This will be exploited in Algorithm 5.4 below. To compute the gradients of the reduced objective function associated with (5.1), we formulate the following corollary of Theorem 4.1:

LEMMA 5.2 (Calculation of Gradients). Denote the solution operator of the lowerlevel problem in (5.1) and the reduced objective function associated with (5.1) with S and F, respectively, i.e.,  $S : \mathbb{R}^n \times (0, \infty) \to \mathbb{R}^n$ ,  $(u, \alpha) \mapsto y$ , and

$$F: \mathbb{R}^n \times (0, \infty) \to \mathbb{R}, \qquad (u, \alpha) \mapsto \frac{1}{2} \left\langle B(y - y_D), y - y_D \right\rangle + \frac{\mu}{2} \left( \left\langle Bu, u \right\rangle + \alpha^2 \right)$$

Then, the gradient  $F'(u, \alpha) \in \mathbb{R}^n \times \mathbb{R}$  at a point  $(u, \alpha) \in \mathbb{R}^n \times (0, \infty)$  with associated state  $y := S(u, \alpha)$  is given by

(5.4) 
$$F'(u,\alpha) = \left( B(\mu u + p), \mu \alpha - \sum_{k:G_k y \neq 0} |T_k| \left( \frac{(G_k y)(G_k p)}{|G_k y|} + \frac{(G_k y)(G_k p)}{\alpha^{1/2} |G_k y|^{1/2}} \right) \right).$$

Here,  $p \in \mathbb{R}^n$  is the unique solution of the variational equality

(5.5) 
$$\begin{cases} p \in W(y), \\ \langle Ap, z \rangle + \sum_{k: G_k y \neq 0} |T_k| \alpha^{1/2} \frac{(G_k p)(G_k z)}{|G_k y|^{1/2}} = \langle B(y - y_D), z \rangle \quad \forall z \in W(y) \end{cases}$$

with  $W(y) := \{ z \in \mathbb{R}^n \mid G_k z = 0 \text{ for all } k = 1, ..., m \text{ with } G_k y = 0 \}.$ 

*Proof.* The claim follows immediately from Theorem 4.1, the self-adjointness of the operators A and B and the chain rule in [5, Proposition 2.47].

Finally, we observe the following:

LEMMA 5.3. The discretized optimal control problem (5.1) admits at least one solution  $(u^*, \alpha^*) \in \mathbb{R}^n \times [\kappa, \infty)$ . Further, every solution  $(u^*, \alpha^*)$  of (5.1) satisfies  $\zeta(u^*, \alpha^*) = 0$ , where  $\zeta : \mathbb{R}^n \times [\kappa, \infty) \to [0, \infty)$  is the function defined by

(5.6) 
$$\zeta(u,\alpha) := \begin{cases} \|F'(u,\alpha)\| & \text{if } \alpha > \kappa, \\ \|\big((\partial_u F)(u,\alpha),\min(0,(\partial_\alpha F)(u,\alpha))\big)\| & \text{if } \alpha = \kappa. \end{cases}$$

*Proof.* To show that the problem (5.1) admits a solution, we can use exactly the same argumentation as in the proof of Theorem 2.1. It remains to prove that  $\zeta(u, \alpha) = 0$  is a necessary optimality condition. This, however, follows immediately from the equivalence

$$\zeta(u,\alpha) = 0 \qquad \Longleftrightarrow \qquad -F'(u,\alpha) \in \mathcal{N}_{\mathbb{R}^n \times [\kappa,\infty)}(u,\alpha),$$

for all  $(u, \alpha) \in \mathbb{R}^n \times [\kappa, \infty)$ , where  $\mathcal{N}_{\mathbb{R}^n \times [\kappa, \infty)}(u, \alpha)$  denotes the normal cone to the set  $\mathbb{R}^n \times [\kappa, \infty)$  at  $(u, \alpha)$ .

We are now in the position to state the algorithm that we use for the solution of the problem (5.1):

Algorithm	<b>5.4</b>	Gradient	Proj	jection	Method	for	the	Solution	of (	(5.1)	)
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Choose an initial guess  $(u_0, \alpha_0) \in \mathbb{R}^n \times [\kappa, \infty)$  and parameters  $\sigma > 0, \nu, \theta \in (0, 1)$ . for  $i = 0, 1, 2, 3, \dots$  do Calculate  $y_i := S(u_i, \alpha_i)$  by solving (5.2) with a semi-smooth Newton method. Calculate  $F_i := F(u_i, \alpha_i)$  and solve (5.5) for  $p_i := p(u_i, \alpha_i)$ . Use the relation (5.4) to assemble the gradient  $F'(u_i, \alpha_i)$ . Calculate the stationarity measure  $\zeta_i := \zeta(u_i, \alpha_i)$  (with  $\zeta$  as in (5.6)). if  $\zeta_i = 0$  then break end if Define  $g_i := (\partial_u F)(u_i, \alpha_i)/\zeta_i$  and  $h_i := (\partial_\alpha F)(u_i, \alpha_i)/\zeta_i$ . Initialize  $\sigma_0 := \sigma$  and calculate a step size as follows: for  $j = 0, 1, 2, 3, \dots$  do Use (5.2) to calculate the quantity  $F_i - F(u_i - \sigma_j g_i, \max(\kappa, \alpha_i - \sigma_j h_i))$  $-\theta\sigma_j\zeta_i\left(\|g_i\|^2 + \min(0,h_i)^2 + \min\left(\max(0,h_i)^2,\max(0,h_i)\frac{(\alpha_i - \kappa)}{\sigma_i}\right)\right)$  $=: e_i.$ if  $e_j < 0$  then

Define  $\sigma_{j+1} := \nu \sigma_j$ . else Define  $\tau_i := \sigma_j$  and break. end if end for Define  $u_{i+1} := u_i - \tau_i g_i$  and  $\alpha_{i+1} := \max(\kappa, \alpha_i - \tau_i h_i)$ . end for

To see that Algorithm 5.4 is sensible, we note the following:

LEMMA 5.5. For every arbitrary but fixed tuple  $(u_i, \alpha_i) \in \mathbb{R}^n \times [\kappa, \infty)$  that satisfies  $\zeta(u_i, \alpha_i) \neq 0$ , and every choice of parameters  $\sigma > 0$  and  $\nu, \theta \in (0, 1)$ , the Armijo-type line-search in Algorithm 5.4 (i.e., the inner for-loop with index j) terminates after finitely many steps.

*Proof.* From the Fréchet differentiability of the reduced objective function F, the definitions  $\zeta_i := \zeta(u_i, \alpha_i), g_i := (\partial_u F)(u_i, \alpha_i)/\zeta_i, h_i := (\partial_\alpha F)(u_i, \alpha_i)/\zeta_i$ , and simple distinctions of cases, it follows straightforwardly that

$$\begin{split} F(u_i, \alpha_i) &- F(u_i - sg_i, \max(\kappa, \alpha_i - sh_i)) \\ &= s\zeta_i \|g_i\|^2 + \zeta_i h_i \left(\alpha_i - \max(\kappa, \alpha_i - sh_i)\right) + o(s) \\ &= \begin{cases} s\zeta_i \|g_i\|^2 + s\zeta_i h_i^2 + o(s) & \text{if } \alpha_i - sh_i \ge \kappa \\ s\zeta_i \|g_i\|^2 + \zeta_i h_i (\alpha_i - \kappa) + o(s) & \text{if } \alpha_i - sh_i < \kappa \end{cases} \\ &= \begin{cases} s\zeta_i \|g_i\|^2 + s\zeta_i \min(0, h_i)^2 + s\zeta_i \max(0, h_i)^2 + o(s) & \text{if } \alpha_i - sh_i \ge \kappa \\ s\zeta_i \|g_i\|^2 + s\zeta_i \min(0, h_i)^2 + \zeta_i \max(0, h_i) (\alpha_i - \kappa) + o(s) & \text{if } \alpha_i - sh_i < \kappa \end{cases} \\ &\ge s\zeta_i \|g_i\|^2 + s\zeta_i \min(0, h_i)^2 + \zeta_i \min(0, h_i)^2, \max(0, h_i) (\alpha_i - \kappa) + o(s) \end{cases} \end{split}$$

holds for all  $s \in (0, \infty)$ , where the Landau symbol refers to the limit  $s \searrow 0$ . Since  $\zeta_i \neq 0$  and, as a consequence,

$$\liminf_{s \searrow 0} \left( \|g_i\|^2 + \min(0, h_i)^2 + \min\left( \max(0, h_i)^2, \max(0, h_i) \frac{(\alpha_i - \kappa)}{s} \right) \right) > 0,$$

the above yields that there exists an  $s_0 > 0$  such that, for all  $s \in (0, s_0)$ , we have

$$F(u_i, \alpha_i) - F(u_i - sg_i, \max(\kappa, \alpha_i - sh_i))$$
  

$$\geq \theta s\zeta_i \left( \|g_i\|^2 + \min(0, h_i)^2 + \min\left(\max(0, h_i)^2, \max(0, h_i)\frac{(\alpha_i - \kappa)}{s}\right) \right)$$

for all  $s \in (0, s_0)$ . This proves the claim.

We may now prove:

THEOREM 5.6 (Convergence Properties of Algorithm 5.4). For every choice of the initial guess  $(u_0, \alpha_0) \in \mathbb{R}^n \times [\kappa, \infty)$  and the parameters  $\sigma > 0$  and  $\nu, \theta \in (0, 1)$ , Algorithm 5.4 either terminates after finitely many steps with an iterate which satisfies the stationarity condition in Lemma 5.3 or produces an infinite sequence of iterates  $\{(u_i, \alpha_i)\}$  with the following properties:

- 1. The sequence of function values  $\{F(u_i, \alpha_i)\}$  is monotonously decreasing.
- 2. The sequence  $\{(u_i, \alpha_i)\}$  is bounded and has at least one accumulation point.
- 3. Every accumulation point  $(u^*, \alpha^*)$  of the sequence  $\{(u_i, \alpha_i)\}$  is stationary in the sense of Lemma 5.3.

*Proof.* The proof is fairly standard. We include it for the convenience of the reader and to demonstrate that, in the situation of the problem (5.1), we do not require the assumption of  $C^{1,1}$ -regularity made, e.g., in [4].

First, we note that Algorithm 5.4 can only terminate after finitely many steps if the exit condition  $\zeta_i = 0$  is triggered (cf. Lemma 5.5). This shows that, if only a finite number of iterates is generated, then the last of these iterates is necessarily stationary in the sense of Lemma 5.3. It remains to study the case where Algorithm 5.4 produces an infinite sequence  $\{(u_i, \alpha_i)\}$ . In this situation, it follows from the sufficient decrease condition that is used for the calculation of the step sizes  $\tau_i$  that the sequence  $\{F(u_i, \alpha_i)\}$  is monotonously decreasing, and we obtain from the structure of the objective function in (5.1) that there exists a constant C > 0 independent of i with

$$0 \le ||(u_i, \alpha_i)||^2 \le CF(u_i, \alpha_i) \le CF(u_0, \alpha_0)$$

The above implies that the sequence  $\{(u_i, \alpha_i)\}$  is bounded, that the function values  $F(u_i, \alpha_i)$  converge for  $i \to \infty$ , and that the sequence  $\{(u_i, \alpha_i)\}$  possesses at least one accumulation point. To prove that every accumulation point of the iterates is stationary in the sense of Lemma 5.3, we argue by contradiction: Suppose that there exists an accumulation point  $(u^*, \alpha^*) \in \mathbb{R}^n \times [\kappa, \infty)$  of the sequence  $\{(u_i, \alpha_i)\}$  which satisfies  $\zeta(u^*, \alpha^*) > 0$ , and let  $(u_{i_i}, \alpha_{i_j})$  be a subsequence with  $(u_{i_i}, \alpha_{i_j}) \to (u^*, \alpha^*)$ for  $j \to \infty$ . Then, it follows from the continuous Fréchet differentiability of F, the definition of the stationarity measure  $\zeta$  and the boundedness of  $\{(u_i, \alpha_i)\}$  that the sequence  $\{\zeta(u_{i_j}, \alpha_{i_j})\} \subset [0, \infty)$  is bounded, and we may assume w.l.o.g. that  $\zeta_{i_j} := \zeta(u_{i_j}, \alpha_{i_j}) \to \zeta^*$  holds for some  $\zeta^* \ge 0$ . Note that we can ignore the case  $\zeta^* = 0$ here since this equality would imply  $\zeta(u^*, \alpha^*) = 0$  (see (5.6), the continuity of F' and a simple distinction of cases). Thus, w.l.o.g.  $\zeta^* > 0$  and  $\zeta_{i_i} \ge \varepsilon > 0$  for some constant  $\varepsilon > 0$ . We now consider two different situations: If there exists a subsequence of  $i_j$ (still denoted by the same symbol) such that the step sizes  $\tau_{i_i} \in (0, \sigma]$  satisfy  $\tau_{i_i} \to \tau^*$ for some  $\tau^* > 0$ , then we obtain from our line-search procedure, the definitions of  $g_{i_i}$ and  $h_{i_i}$ , the convergence of the function values  $\{F(u_i, \alpha_i)\}$  and the continuity of the derivative F' that

$$0 = \lim_{j \to \infty} \left( F(u_{i_j}, \alpha_{i_j}) - F(u_{i_j+1}, \alpha_{i_j+1}) \right)$$
  

$$\geq \lim_{j \to \infty} \theta \tau_{i_j} \zeta_{i_j} \left( \|g_{i_j}\|^2 + \min(0, h_{i_j})^2 + \min\left(\max(0, h_{i_j})^2, \max(0, h_{i_j}) \frac{(\alpha_{i_j} - \kappa)}{\tau_{i_j}}\right) \right)$$
  

$$\geq \frac{\theta \tau^*}{\zeta^*} \left( \|(\partial_u F)(u^*, \alpha^*)\|^2 + \min(0, (\partial_\alpha F)(u^*, \alpha^*))^2 + \min\left(\max(0, (\partial_\alpha F)(u^*, \alpha^*)) \frac{(\alpha^* - \kappa)\zeta^*}{\tau^*}\right) \right)$$
  

$$\geq 0.$$

The above implies  $\zeta(u^*, \alpha^*) = 0$  which is a contradiction. It remains to consider the case where the step sizes  $\tau_{i_j}$  converge to zero for  $j \to \infty$ . In this situation, it follows from our line-search algorithm and the mean value theorem that, for all sufficiently large j, we have (5.7)

$$F(u_{i_j}, \alpha_{i_j}) - F\left(u_{i_j} - \frac{\tau_{i_j}}{\nu}g_{i_j}, \max\left(\kappa, \alpha_{i_j} - \frac{\tau_{i_j}}{\nu}h_{i_j}\right)\right)$$

$$= \int_0^1 \left\langle F'\left(u_{i_j} - s\frac{\tau_{i_j}}{\nu}g_{i_j}, \alpha_{i_j} - s\left(\alpha_{i_j} - \max\left(\kappa, \alpha_{i_j} - \frac{\tau_{i_j}}{\nu}h_{i_j}\right)\right)\right)$$

$$, \left(\frac{\tau_{i_j}}{\nu}g_{i_j}, \alpha_{i_j} - \max\left(\kappa, \alpha_{i_j} - \frac{\tau_{i_j}}{\nu}h_{i_j}\right)\right)\right) \right\rangle ds$$

$$\leq \frac{\theta \tau_{i_j} \zeta_{i_j}}{\nu} \left( \|g_{i_j}\|^2 + \min(0, h_{i_j})^2 + \min\left(\max(0, h_{i_j})^2, \max(0, h_{i_j})\frac{(\alpha_{i_j} - \kappa)\nu}{\tau_{i_j}}\right)\right) \right)$$

If we assume that there exists a subsequence of  $i_j$  (again not relabeled) such that  $\alpha_{i_j} - \tau_{i_j} h_{i_j} / \nu \geq \kappa$  holds for all j, then we may divide the left- and the right-hand side of (5.7) by  $\tau_{i_j}$ , employ the elementary estimate  $\min(a, b) \leq a$  for all  $a, b \in \mathbb{R}$ , and pass to the limit  $j \to \infty$  (using the continuity of the derivative F', the boundedness of the iterates  $\{(u_i, \alpha_i)\}$ , the definitions of  $g_{i_j}$  and  $h_{i_j}$ , the convergence  $\tau_{i_j} \searrow 0$ , and the dominated convergence theorem) to obtain

$$\frac{1}{\zeta^*\nu} \|F'(u^*, \alpha^*)\|^2 \le \frac{\theta}{\zeta^*\nu} \|F'(u^*, \alpha^*)\|^2.$$

This inequality again contradicts our assumption  $\zeta(u^*, \alpha^*) > 0$ . If, on the other hand, we can find a subsequence of  $i_j$  with  $\alpha_{i_j} - \tau_{i_j} h_{i_j} / \nu \leq \kappa$ , then, along this subsequence, it necessarily holds

(5.8) 
$$0 \le \frac{\alpha_{i_j} - \kappa}{\tau_{i_j}} \le \frac{1}{\nu} h_{i_j}, \qquad \alpha_{i_j} \to \kappa = \alpha^* \quad \text{and} \quad h_{i_j} \to \frac{(\partial_\alpha F)(u^*, \alpha^*)}{\zeta^*} \ge 0,$$

and we may assume w.l.o.g. that  $(\alpha_{i_j} - \kappa)/\tau_{i_j} \to \xi$  holds for some  $\xi \ge 0$ . By dividing by  $\tau_{i_j}$  in (5.7) and by passing to the limit  $j \to \infty$ , we now obtain analogously to the case  $\alpha_{i_j} - \tau_{i_j} h_{i_j}/\nu \ge \kappa$  that

$$\begin{split} &\frac{1}{\zeta^*\nu} \|(\partial_u F)(u^*,\alpha^*)\|^2 + \xi(\partial_\alpha F)(u^*,\alpha^*) \\ &\leq \frac{\theta}{\zeta^*\nu} \|(\partial_u F)(u^*,\alpha^*)\|^2 + \min\left(\frac{\theta}{\zeta^*\nu}(\partial_\alpha F)(u^*,\alpha^*)^2, \theta\xi(\partial_\alpha F)(u^*,\alpha^*)\right) \\ &\leq \theta\left(\frac{1}{\zeta^*\nu} \|(\partial_u F)(u^*,\alpha^*)\|^2 + \xi(\partial_\alpha F)(u^*,\alpha^*)\right). \end{split}$$

The above implies  $\|(\partial_u F)(u^*, \alpha^*)\|^2 = 0$  and yields, in combination with (5.8) and the definition of  $\zeta$ , that  $\zeta(u^*, \alpha^*) = 0$ . This is again a contradiction. Accumulation points with  $\zeta(u^*, \alpha^*) > 0$  thus cannot exist and the proof is complete.

The results of a numerical experiment conducted with Algorithm 5.4 can be seen in Figure 2 below. As the plots show, the behavior of the iterates generated by our gradient projection method accords very well with the predictions of Theorem 5.6. In particular, we observe that the quantity  $\zeta_i := \zeta(u_i, \alpha_i)$ , which measures the degree of stationarity of the current iterate  $(u_i, \alpha_i)$ , converges to zero as *i* tends to infinity. This demonstrates that Theorems 3.3 and 4.1 indeed make it possible to solve bilevel optimization problems of the type (P) with standard gradient-based algorithms. We would like to emphasize at this point that Algorithm 5.4 solves (5.1) "as it is", i.e., in the presence of the absolute value functions on the lower level and without any kind of regularization or modification of the problem or the solution procedure (in contrast to the methods in [8, 15, 20, 28, 35, 36]). The latter implies in particular that the sparsity promoting effects that the non-smooth terms  $|G_k(\cdot)|$  in (5.1) have on the gradient of the finite element functions  $\bar{y}_h^* := \sum y_j^* \varphi_j$ ,  $\bar{p}_h^* := \sum p_j^* \varphi_j$  and  $\bar{u}_h^* := \sum u_j^* \varphi_j$  associated with a solution  $(u^*, \alpha^*) \in \mathbb{R}^n \times [\kappa, \infty)$  of (5.1) (cf. Section 2.1) are preserved in our approach. This can also be seen in Figure 2 where the optimal state  $\bar{y}_h^* \in V_h$  has a distinct "flat" region in the middle of the fluid domain. Recall that, in the context of the optimal control problem (5.1), the set  $\{\nabla \bar{y}_h^* = 0\}$  is exactly that part of the domain  $\Omega$  where the viscoplastic medium under consideration behaves like a solid (the nucleus). Our solution method thus allows to identify precisely where rigid material behavior occurs in the fluid domain when we optimize the objective function in (5.1). Such an identification is not possible anymore when regularization approaches are used which necessarily remove the sparsity promoting effects from the problem. Note that the functions  $\bar{p}_h^* \in V_h$  and  $\bar{u}_h^* \in V_h$  associated with a solution  $(u^*, \alpha^*)$  of (5.1) directly inherit the "flatness" properties of  $\bar{y}_h^*$  due to (5.5) and since the optimality condition  $\zeta(u^*, \alpha^*) = 0$  implies  $\mu u^* + p^* = 0$ , see (5.4).



FIG. 2. Numerical results obtained for the problem (5.1) on the interval  $\Omega = (0,1)$  with an equidistant partition  $\mathcal{T}$  of width 1/500 and  $\mu = 0.000025$ ,  $\kappa = 3$ ,  $\sigma = 40$ ,  $\nu = 0.25$ ,  $\theta = 0.5$ ,  $\alpha_0 = 4$  and  $u_0 = (10, 10, ..., 10)$ . Figures (a) and (b) show the reduction of the function value  $F_i$  and the stationarity measure  $\zeta_i$  during the first 200 iterations of Algorithm 5.4. The state, the control, the multipliers and the adjoint state of the approximate solution at iteration 200 can be seen in figures (c) to (f). The considered desired state  $\bar{y}_D \in H_0^1(\Omega)$  is plotted as a dashed line in (c). The multipliers  $\lambda_k^*$  are depicted as a step function whose value on a cell  $T_k$  of  $\mathcal{T}$  is  $\lambda_k$ . As a tolerance for the residue of the semi-smooth Newton method used for the solution of (5.2), we chose  $10^{-10}$ .

We conclude this paper with some additional remarks on Algorithm 5.4, the numerical results in Figure 2, and the analysis in Sections 3 and 4:

Remark 5.7.

- 1. As the graph in Figure 2(a) shows, in our numerical experiment, we do not observe a significant decrease of the function value  $F_i$  anymore after approximately 25 gradient steps. This number of iterations is thus sufficient if we are primarily interested in determining a tuple  $(u, \alpha)$  for which the value of the reduced objective function is as small as possible. We would like to point out that, although  $F_i$  remains nearly constant for  $i \ge 25$ , the stationarity measure  $\zeta_i$  still changes in the later iterations of the algorithm. The same is true for the quantities  $u_i$  and  $p_i$ . The two global maxima of the control seen in Figure 2(d), for example, are not visible until  $i \approx 60$ .
- 2. In the numerical experiment of Figure 2, the Oldroyd number  $\alpha$  is decreased from the initial guess  $\alpha_0 = 4$  to the lower bound  $\kappa = 3$  in the first three iterations of Algorithm 5.4 and afterwards remains constant. This makes sense since a low  $\alpha$  is preferable in the situation of the discrete tracking-type optimal control problem (5.1). (The lower the material parameter  $\alpha$ , the lower the yield stress and the smaller the pressure gradient that is needed to create a desired flow profile.) If we replace the term  $\alpha^2$  on the upper level of (5.1) with, e.g.,  $(\alpha - \alpha_D)^2$  for some sufficiently large  $\alpha_D > 0$ , then this behavior changes and we observe convergence to an  $\alpha^* > \kappa$ .
- 3. It is easy to check that the solution operator  $S : \mathbb{R}^n \times (0, \infty) \to \mathbb{R}^n$  associated with the elliptic variational inequality on the lower level of (5.1) is constant zero in an open neighborhood of the cone  $\{0\} \times (0, \infty)$ . (This is precisely the set where the pressure gradient is not large enough to move the fluid under consideration, compare also with (3.13).) Because of this behavior, the tuple  $(0, \kappa)$  is always a local minimizer of (5.1) and a stationary point in the sense of Lemma 5.3. To avoid converging to the point  $(0, \kappa)$ , which is typically not globally optimal and thus only of limited interest, one has to choose an initial guess  $u_0$  that is sufficiently far away from the origin when an iterative method analogous to Algorithm 5.4 is used for the solution of (5.1). Note that, in the situation of Figure 2, we have indeed found a point that is better than  $(0, \kappa)$  since the final iterate achieves a function value that is far smaller than  $F(0, \kappa) \approx 0.333446$ .
- 4. Note that the variational problems (4.1) and (5.5) can also be formulated as quadratic minimization problems with linear equality constraints. This makes it possible to use standard methods from quadratic programming for the calculation of the adjoint state and the gradient of the reduced objective function. In the numerical experiment of Figure 2, we determined p with the Matlab routine quadprog.
- 5. We would like to point out that, if an iterative scheme is used for the solution of the lower-level problem in (5.1), then the successive evaluations of the maps S and F in the line-search procedure of Algorithm 5.4 can be performed quite effectively since the last trial iterate can always be used as an initial guess for the calculation of the next required state  $S(u_i - \sigma_j g_i, \max(\kappa, \alpha_i - \sigma_j h_i))$ . In the situation of Figure 2, it can be observed that Algorithm 5.4 requires an average of approximately four evaluations of the solution operator S per gradient step over the first 200 iterations. The majority of these calculations are needed for large i.

- 6. In this section, we have considered Algorithm 5.4 as a stand-alone solution procedure for the bilevel optimization problem (5.1). This is, of course, not necessary. We could have also combined our algorithm with an inaccurate but cheap method (e.g., a regularization approach) that provides a good initial guess  $(u_0, \alpha_0)$ . Such a technique has been used, e.g., in [11, Section 5].
- 7. Alternatively to the approach that we have pursued in this section, one could also try to tackle the necessary optimality condition  $\zeta(u^*, \alpha^*) = 0$  in Lemma 5.3 directly, e.g., with a Newton-type method or a primal-dual-active-set-type algorithm. (Note that some care has to be taken here since Theorem 3.3 only provides a first derivative but not a second one so that a classical Newton algorithm is out of question.) We leave this topic for further research.

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